

Chapter 9 - COHERENT AND INCOHERENT NEUTRON SCATTERING

Neutron scattering is characterized by coherent and incoherent contributions to scattering. Coherent scattering depends on Q and is therefore the part that contains information about scattering structures, whereas SANS incoherent scattering is featureless (Q independent) and contains information about the material scattering density only. Here only elastic scattering is considered.

1. COHERENT AND INCOHERENT CROSS SECTIONS

The coherent and incoherent parts of the elastic scattering cross section are separated. Consider a set of N nuclei with scattering lengths b_i in the sample. The scattering cross section is given by:

$$\frac{d\sigma(\theta)}{d\Omega} = |f(\theta)|^2 = \left(\frac{m}{2\pi\hbar^2} \right)^2 \left| \int d\vec{r} \exp(-i\vec{Q}\cdot\vec{r}) V(r) \right|^2. \quad (1)$$

Here $f(\theta)$ is the scattering amplitude, $\vec{Q} = \vec{k}_s - \vec{k}_i$ is the scattering vector and $V(r)$ is the Fermi pseudopotential describing neutron-nucleus interactions:

$$V(r) = \left(\frac{2\pi\hbar^2}{m} \right) \sum_{i=1}^N b_i \delta(\vec{r} - \vec{r}_i). \quad (2)$$

Here \vec{r}_i is the position and b_i the scattering length of nucleus i . Therefore, the differential scattering cross section is the sum of the various scattering phases from all of the nuclei in the sample properly weighed by their scattering lengths:

$$\frac{d\sigma(\theta)}{d\Omega} = \sum_{i=1}^N \sum_{j=1}^N b_i b_j \langle \exp(i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)) \rangle \quad (3)$$

where $\langle \dots \rangle$ represents an “ensemble” average (i.e., average over scatterers’ positions and orientations).

Consider an average over a set consisting of a number m of nuclei:

$$\{ \dots \} = \frac{1}{m} \sum_{i=1}^m \dots \quad (4)$$

This average could be over different atoms, over different isotopes or different atoms in a small molecule.

Define average and fluctuating parts for the scattering lengths $b_i = \{b\} + \delta b_i$ and positions $\vec{r}_i = \vec{R}_\alpha + \vec{S}_{\alpha i}$ as well as the following:

- $\vec{R}_{\alpha i}$: position of the center-of-mass of molecule α
- $\vec{S}_{\alpha i}$: relative position of scatterer i inside molecule α
- m : number of nuclei per molecule
- M : number of molecules in the sample (Note that $N = mM$).

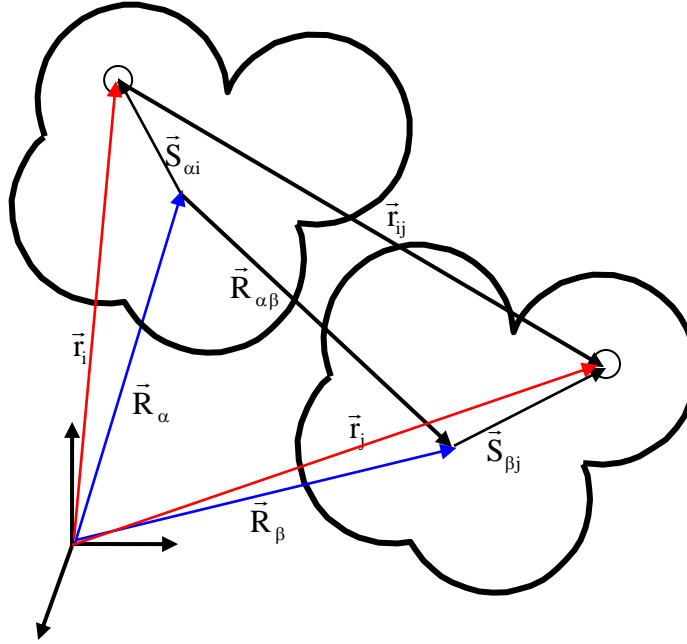


Figure 1: Parametrization for two scattering molecules.

The various terms of the scattering cross section can be separated as:

$$\frac{d\sigma(\theta)}{d\Omega} = \sum_{i,j}^N [\{b\} + \delta b_i] [\{b\} + \delta b_j] \langle \exp(i\vec{Q} \cdot (\vec{r}_i - \vec{r}_j)) \rangle \quad (5)$$

$$\frac{d\sigma(\theta)}{d\Omega} = \{b\}^2 \sum_{i,j}^N \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle + \sum_{i,j}^N \delta b_i \delta b_j \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle + 2\{b\} \sum_{i,j}^N \delta b_i \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle$$

where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. If \vec{r}_{ij} is approximated by $\vec{R}_{\alpha\beta}$ which is equivalent to $S_{\alpha i} \ll R_\alpha$ (all nuclei of one molecule are located very close to each other) the term:

$$\sum_i^N \delta b_i \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle \cong \left(\sum_i^N \delta b_i \right) \langle \exp(i\vec{Q} \cdot \vec{R}_{\alpha\beta}) \rangle = 0 \quad (6)$$

can be neglected. This is due to the definition of the center-of-mass $\{\delta b_i\} = \sum_i^N \delta b_i = 0$.

The term $\sum_{i,j}^N \delta b_i \delta b_j \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle$ contributes only when $i=j$. When $i \neq j$,

$$\sum_{i,j}^N \delta b_i \delta b_j \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle \cong \left(\sum_i^N \delta b_i \right) \left(\sum_j^N \delta b_j \right) \langle \exp(i\vec{Q} \cdot \vec{R}_{\alpha\beta}) \rangle = 0.$$

Therefore, the scattering cross section can be written simply as the sum of two contributions:

$$\begin{aligned} \frac{d\sigma(\theta)}{d\Omega} &= \{b\}^2 \sum_{i,j}^N \langle \exp(i\vec{Q} \cdot \vec{r}_{ij}) \rangle + \sum_{i,j}^N \delta b_i^2 \\ &= \left[\frac{d\sigma(\theta)}{d\Omega} \right]_{\text{coh}} + \left[\frac{d\sigma(\theta)}{d\Omega} \right]_{\text{inc}}. \end{aligned} \quad (7)$$

The last term is the **incoherent cross section** for the whole sample:

$$\left[\frac{d\sigma(\theta)}{d\Omega} \right]_{\text{inc}} = \{\delta b^2\} = \{b^2\} - \{b\}^2. \quad (8)$$

Note that these are cross sections per atom. Cross sections can also be defined per molecule instead as $m \frac{d\sigma(\theta)}{d\Omega}$ where m is the number of atoms per molecule.

Incoherent scattering has two contributions: one from spin incoherence (different atoms) **and the other from isotopic incoherence** (different isotopes). Disorder scattering (different atoms in a small molecule) could be considered as coherent (not incoherent) scattering even though it is Q -independent in the SANS range due to the smallness of the molecules. Note that in x-ray scattering, there is no equivalent for spin-incoherence and that contributions from disorder scattering are coherent. Spin-incoherence, isotopic incoherence and disorder scattering will be described in the next sections.

2. SPIN INCOHERENCE

Nuclei with nonzero spin contribute to spin incoherence since neutron and nuclear spins could be either parallel or antiparallel during the scattering process. **The neutron is a Fermion with spin 1/2** which **couple to the nuclear spin I** to give:

- $2I + 2$ states (for which the scattering length is noted b_+) corresponding to parallel neutron and nuclear spins, or
- $2I$ states (for which the scattering length is noted b_-) corresponding to antiparallel neutron and nuclear spins.

There are $2(2I + 1)$ total states with the following weighing factors:

$$W_+ = \frac{(2I+2)}{2(2I+1)} = \frac{I+1}{2I+1} \text{ and } W_- = \frac{2I}{2(2I+1)} = \frac{I}{2I+1}. \quad (9)$$

Note that $W_+ + W_- = 1$. In the case of the hydrogen nucleus ($I = 1/2$), W_+ corresponds to a triplet state and W_- corresponds to a singlet state.

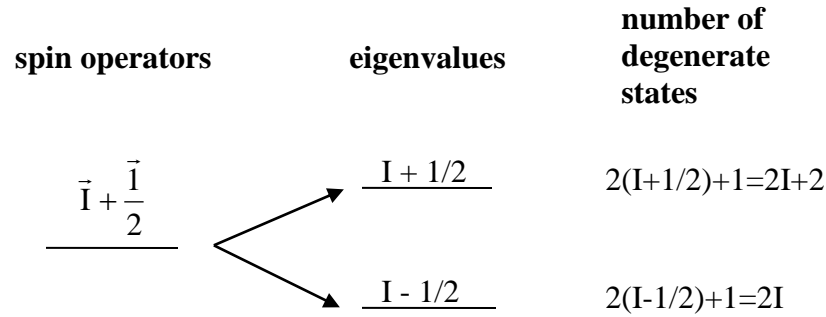


Figure 2: Representation of the neutron spin $1/2$ with its up and down values and the nuclear spin \vec{I} .

The averages over spin states are calculated for coherent and spin-incoherent scatterings using:

$$\begin{aligned} \{b\} &= W_+ b_+ + W_- b_- = \frac{(I+1)b_+ + Ib_-}{2I+1} \\ \{b^2\} &= W_+ b_+^2 + W_- b_-^2 = \frac{(I+1)b_+^2 + Ib_-^2}{2I+1}. \end{aligned} \quad (10)$$

Either the two scattering lengths b_+ and b_- or the other two scattering lengths b_c and b_i could be tabulated for each (isotope) element. Most often, it is the b_c and b_i scattering lengths that are tabulated. Tables are based on measurements made using thermal neutrons.

$$\begin{aligned} b_c &= \{b\} = W_+ b_+ + W_- b_- \\ b_i &= \sqrt{\{b^2\} - \{b\}^2} = \sqrt{W_+ W_-} (b_+ - b_-). \end{aligned} \quad (11)$$

For the scattering from **hydrogen** (pure H-1) nuclei:

$$b_c = -3.7406 \text{ fm}, b_i = 25.274 \text{ fm}, \sigma_c = 1.7583 \text{ barn}, \sigma_i = 80.27 \text{ barn}.$$

The corresponding **microscopic cross sections** are obtained as $\sigma_c = 4\pi b_c^2$ and $\sigma_i = 4\pi b_i^2$.

The b_+ and b_- scattering lengths can be calculated from b_c and b_i as follows:

$$\begin{aligned} b_+ &= b_c + \sqrt{\frac{W_-}{W_+}} b_i = b_c + \sqrt{\frac{I}{I+1}} b_i \\ b_- &= b_c - \sqrt{\frac{W_+}{W_-}} b_i = b_c - \sqrt{\frac{I+1}{I}} b_i. \end{aligned} \quad (12)$$

For hydrogen ($I=1/2$), $b_+ = 10.851 \text{ fm}$ and $b_- = -47.517 \text{ fm}$. A **spin-dependent scattering length** is expressed in terms of the neutron and nuclear spin operators \vec{s} and \vec{I} as:

$$b_c + \frac{2\vec{s} \cdot \vec{I}}{\sqrt{I(I+1)}} b_i. \quad (13)$$

In order **to separate out the coherent and incoherent components**, three options present themselves. (1) **Use of polarized neutrons along with polarization analysis**. Polarization analysis is not easy to achieve due to the large divergence angles in the SANS scattered beam. (2) **Aligning the nuclear spins** along with using polarized neutrons. Aligning nuclear spins is extremely difficult and has not matured to be a viable alternative. Note that the **field of magnetism involves aligning electron (not nuclear) spins**. (3) **Using deuterium labeling**. Deuterium labeling is used routinely to minimize the incoherent signal from hydrogen atoms (deuterium has a low incoherent component).

3. COHERENT SCATTERING CROSS SECTION

The **coherent scattering cross section** is given by the integral of the differential cross section over solid angle:

$$\sigma_c = \int \frac{d\sigma_c}{d\Omega} d\Omega.$$

Consider **the case of a generic molecule $A_m B_n$ made out of m atoms of element A and n atoms of element B**. Define the **number fractions $f_A = m/(m+n)$ and $f_B = n/(m+n)$** obeying $f_A + f_B = 1$. The **coherent scattering cross section per atom** for molecule $A_m B_n$ is given by:

$$\sigma_c(A_m B_n) = 4\pi \{b\}^2 = 4\pi (f_A b_A + f_B b_B)^2. \quad (14)$$

Consider the case of water (H_2O) with $b_{\text{H}} = -3.739$ fm, $b_{\text{O}} = 5.803$ fm, $f_{\text{H}} = 2/3$ and $f_{\text{O}} = 1/3$ yielding $\sigma_{\text{c}}(\text{H}_2\text{O}) = 4\pi(-2 \cdot 3.739/3 + 5.803/3)^2 \text{ fm}^2 = 0.039$ barn. Note that $b_{\text{H}} = -3.739$ fm for hydrogen with natural abundance of H-1, H-2 (D), and H-3 (T), whereas $b_{\text{H}} = -3.7406$ fm for pure H-1. Recall that 1 barn = 10^{-24} cm^2 and 1 fm = 10^{-13} cm . This is the cross section per atom. The cross section per H_2O molecule is $3 \cdot 0.039 = 0.117$ barn.

Similarly, for heavy water (D_2O) with $b_{\text{D}} = 6.671$ fm, one obtains $\sigma_{\text{c}}(\text{D}_2\text{O}) = 5.12$ barn. The cross section per D_2O molecule is $3 \cdot 5.12 = 15.35$ barn.

4. INCOHERENT SCATTERING AND DISORDER SCATTERING CROSS SECTIONS

Every element in the periodic table has a spin incoherence scattering cross section except if the nuclear spin is zero. Mixing isotopes contributes isotopic incoherence as well. Isotopic incoherence and disorder scattering are lumped into “composition incoherence” since the same formalism is used to estimate them.

Consider the A_mB_n molecule again.

The spin incoherence cross section per atom for the A_mB_n mixture is given by:

$$[\sigma_{\text{i}}(\text{A}_m\text{B}_n)]_{\text{spin}} = f_{\text{A}}\sigma_{\text{i}}(\text{A}) + f_{\text{B}}\sigma_{\text{i}}(\text{B}). \quad (15)$$

The isotopic incoherence and “disorder” scattering cross sections per atom involve the following difference:

$$[\sigma_{\text{i}}(\text{A}_m\text{B}_n)]_{\text{comp}} = 4\pi(\{b^2\} - \{b\}^2). \quad (16)$$

The two averages are $\{b\} = f_{\text{A}}b_{\text{A}} + f_{\text{B}}b_{\text{B}}$ and $\{b^2\} = f_{\text{A}}b_{\text{A}}^2 + f_{\text{B}}b_{\text{B}}^2$. Therefore:

$$\begin{aligned} [\sigma_{\text{i}}(\text{A}_m\text{B}_n)]_{\text{comp}} &= 4\pi[f_{\text{A}}b_{\text{A}}^2 + f_{\text{B}}b_{\text{B}}^2 - (f_{\text{A}}b_{\text{A}} + f_{\text{B}}b_{\text{B}})^2] \\ &= 4\pi f_{\text{A}}f_{\text{B}}(b_{\text{A}} - b_{\text{B}})^2. \end{aligned} \quad (17)$$

Putting both contributions together, the incoherent cross section per atom is obtained as:

$$\sigma_{\text{i}}(\text{A}_m\text{B}_n) = f_{\text{A}}\sigma_{\text{i}}(\text{A}) + f_{\text{B}}\sigma_{\text{i}}(\text{B}) + 4\pi f_{\text{A}}f_{\text{B}}(b_{\text{A}} - b_{\text{B}})^2. \quad (18)$$

Note that the incoherent cross section per molecule is obtained by multiplying by the number of atoms per molecule ($m+n$).

Consider the case of water (H_2O):

$$\sigma_i(\text{H}_2\text{O}) = f_H \sigma_i(\text{H}) + f_O \sigma_i(\text{O}) + 4\pi f_H f_O (b_H - b_O)^2. \quad (19)$$

Using $\sigma_i(\text{H}) = 80.27$ barn, $\sigma_i(\text{O}) = 0$ barn, $b_H = -3.739$ fm, $b_O = 5.803$ fm, $f_H = 2/3$ and $f_O = 1/3$, the following result is obtained $\sigma_i(\text{H}_2\text{O}) = 53.5 + 2.54 = 56.04$ barn. This is the cross section per atom. The cross section per H_2O molecule is $3 \times 56.04 = 168.12$ barn.

Similarly, for heavy water (D_2O). Using $\sigma_i(\text{D}) = 2.05$ barn and $b_D = 6.671$ fm, the following result is obtained $\sigma_i(\text{D}_2\text{O}) = 1.37 + 0.021 = 1.39$ barn. This is the cross section per atom. The cross section per D_2O molecule is $3 \times 1.39 = 4.17$ barn.

Note that in both cases the spin incoherence cross section (first term in units of barn) dominates over the composition incoherence cross section (second term in units of fm^2).

5. TOTAL SCATTERING CROSS SECTION

The total scattering cross section is the sum of the coherent and incoherent contributions.

$$\sigma_s(\text{A}_m\text{B}_n) = \sigma_c(\text{A}_m\text{B}_n) + \sigma_i(\text{A}_m\text{B}_n) \quad (20)$$

$$= 4\pi\{b^2\} + f_A \sigma_i(\text{A}) + f_B \sigma_i(\text{B})$$

$$= 4\pi[f_A b_A^2 + f_B b_B^2] + f_A \sigma_i(\text{A}) + f_B \sigma_i(\text{B}).$$

The first term $\{b^2\}$ contains both coherent and composition incoherence contributions and the other two terms contain the spin incoherence contribution.

For the cases of H_2O and D_2O , one obtains $\sigma_s(\text{H}_2\text{O}) = 56.08$ barn and $\sigma_s(\text{D}_2\text{O}) = 6.51$ barn respectively. These are the cross sections per atom. The cross sections per molecule are $3 \times 56.08 = 168.24$ barn and $3 \times 6.51 = 19.53$ barn.

6. SCATTERING LENGTH DENSITY

What is needed to calculate neutron contrast factors is the scattering length density (not the scattering length). The scattering length density is defined as the ratio of the scattering length per molecule and the molecular volume. Assuming an A_mB_n molecule, the scattering length density is given by:

$$\rho_{\text{AmBn}} = \left(\frac{b}{v} \right)_{\text{AmBn}} = \frac{(f_A b_A + f_B b_B)(m+n)}{v} = \frac{mb_A + nb_B}{v}. \quad (21)$$

Here $mb_A + nb_B$ is the scattering length per molecule and v is the volume of molecule A_mB_n comprising m atoms A and n atoms B.

The molecular volume v is given in terms of the density d and molar mass m for molecule A_mB_n and Avogadro's number N_{av} ($N_{av} = 6 \cdot 10^{23} / \text{mol}$) as:

$$v = \frac{m}{N_{av} d} . \quad (22)$$

For H_2O the density is $d = 1 \text{ g/cm}^3$, the molar mass is $m = 18 \text{ g/mol}$ so that the molecular volume is $v = 3 \cdot 10^{-23} \text{ cm}^3$ and $(b/v)_{H_2O} = -5.58 \cdot 10^9 \text{ cm}^{-2} = -5.58 \cdot 10^{-7} \text{ \AA}^{-2}$. For D_2O , $d = 1.11 \text{ g/cm}^3$, $m = 20 \text{ g/mol}$ so that $v = 3 \cdot 10^{-23} \text{ cm}^3$ and $(b/v)_{D_2O} = 6.38 \cdot 10^{-10} \text{ cm}^{-2} = 6.38 \cdot 10^{-6} \text{ \AA}^{-2}$.

7. CONTRAST FACTORS

The scattering intensity is proportional to the contrast factor. Consider the simple case of scattering inhomogeneities consisting of A molecules in a background of B molecules (think polymers, proteins or micelles in solution). The scattering length densities are (b_A/v_A) and (b_B/v_B) . The contrast factor often referred to as $\Delta\rho^2$ is defined as:

$$\Delta\rho^2 = (\rho_A - \rho_B)^2 = \left(\frac{b_A}{v_A} - \frac{b_B}{v_B} \right)^2 .$$

Scattering length densities can be changed through the deuteration process. Adjusting the relative amount of deuterated to non-deuterated solvent is called a contrast variation series and yields the zero contrast condition whereby the scattering length density of the mixed solvent matches that of the scattering inhomogeneities.

8. MACROSCOPIC SCATTERING CROSS SECTIONS

Keeping the same notation for molecule A_mB_n , the macroscopic scattering cross section Σ is the product of the microscopic cross section per molecule $\sigma(m+n)$ times the number of molecules per unit volume N/V . N is the total number of molecules and V is the total sample volume. For a sample comprising pure A_mB_n substance, $V/N = v$ is the molecular volume. This applies to coherent σ_c , incoherent σ_i or total scattering σ_s cross sections.

$$\Sigma_c = \left(\frac{N}{V} \right) \sigma_c (m+n) \quad (23)$$

$$\Sigma_i = \left(\frac{N}{V} \right) \sigma_i (m+n)$$

$$\Sigma_s = \left(\frac{N}{V} \right) \sigma_s (m+n) .$$

The number density of molecules is given in terms of the density d and molar mass m for molecule A_mB_n and Avogadro's number N_{av} as:

$$\left(\frac{N}{V}\right) = \frac{N_{av}d}{m}. \quad (24)$$

For H_2O , the macroscopic scattering cross sections per molecule are

$$\begin{aligned} \Sigma_c(H_2O) &= \frac{0.117 * 10^{-24}}{3 * 10^{-23}} = 3.9 * 10^{-3} \text{ cm}^{-1} \\ \Sigma_i(H_2O) &= \frac{168.12 * 10^{-24}}{3 * 10^{-23}} = 5.6 \text{ cm}^{-1} \\ \Sigma_s(H_2O) &= \frac{168.24 * 10^{-24}}{3 * 10^{-23}} = 5.6 \text{ cm}^{-1}. \end{aligned}$$

For D_2O , the macroscopic scattering cross sections per molecule are

$$\begin{aligned} \Sigma_c(D_2O) &= \frac{15.35 * 10^{-24}}{3 * 10^{-23}} = 0.512 \text{ cm}^{-1} \\ \Sigma_i(D_2O) &= \frac{4.17 * 10^{-24}}{3 * 10^{-23}} = 0.139 \text{ cm}^{-1} \\ \Sigma_s(D_2O) &= \frac{19.53 * 10^{-24}}{3 * 10^{-23}} = 0.651 \text{ cm}^{-1}. \end{aligned}$$

The results for H_2O and D_2O are summarized next.

9. SUMMARY FOR H_2O AND D_2O

For the case of H_2O

Coherent cross section per atom $\sigma_c(H_2O) = 0.039$ barn.

Coherent cross section per H_2O molecule is $3 * \sigma_c(H_2O) = 0.117$ barn.

Incoherent cross section per atom $\sigma_i(H_2O) = 53.51 + 2.54 = 56.04$ barn

Incoherent cross section per molecule is $3 * \sigma_i(H_2O) = 168.12$ barn.

Total scattering cross section per atom $\sigma_s(H_2O) = 56.08$ barn

Total scattering cross section per molecule is $3 * \sigma_s(H_2O) = 168.24$ barn

Molecular volume $v = 3 * 10^{-23} \text{ cm}^3$

Scattering length density $(b/v)_{H_2O} = -5.58 * 10^{-7} \text{ Å}^{-2}$

Macroscopic coherent cross section $\Sigma_c(\text{H}_2\text{O}) = 3.9 \times 10^{-3} \text{ cm}^{-1}$

Macroscopic incoherent cross section $\Sigma_i(\text{H}_2\text{O}) = 5.604 \text{ cm}^{-1}$

Macroscopic total cross section $\Sigma_s(\text{H}_2\text{O}) = 5.608 \text{ cm}^{-1}$

Table 1: Scattering lengths and cross sections (per atom) for water. In order to obtain cross sections per molecule, one has to multiply by the number of atoms per molecule (i.e., by 3).

		Mixing Fraction	b Fermi	σ_c Barn	$\sigma_{i\text{-spin}}$ Barn	$\sigma_{i\text{-comp}}$ Barn	σ_i Barn	σ_s Barn
Hydrogen	H	2/3	-3.739	-----	80.27	-----	-----	-----
Oxygen	O	1/3	5.803	-----	0	-----	-----	-----
Water	H ₂ O	1	-0.558	0.039	53.51	2.54	56.04	56.08

For the case of D₂O

Coherent cross section per atom $\sigma_c(\text{D}_2\text{O}) = 5.12 \text{ barn}$.

Coherent cross section per D₂O molecule is $3 \times \sigma_c(\text{D}_2\text{O}) = 15.35 \text{ barn}$.

Incoherent cross section per atom $\sigma_i(\text{D}_2\text{O}) = 1.37 + 0.021 = 1.39 \text{ barn}$

Incoherent cross section per molecule is $3 \times \sigma_i(\text{D}_2\text{O}) = 4.17 \text{ barn}$.

Total scattering cross section per atom $\sigma_s(\text{D}_2\text{O}) = 6.51 \text{ barn}$

Total scattering cross section per molecule is $3 \times \sigma_s(\text{D}_2\text{O}) = 19.53 \text{ barn}$

Molecular volume $v = 3 \times 10^{-23} \text{ cm}^3$

Scattering length density $(b/v)_{\text{D}_2\text{O}} = 6.38 \times 10^{-6} \text{ \AA}^{-2}$

Macroscopic coherent cross section $\Sigma_c(\text{D}_2\text{O}) = 0.512 \text{ cm}^{-1}$

Macroscopic incoherent cross section $\Sigma_i(\text{D}_2\text{O}) = 0.139 \text{ cm}^{-1}$

Macroscopic total cross section $\Sigma_s(\text{D}_2\text{O}) = 0.651 \text{ cm}^{-1}$

Table 2: Scattering lengths and cross sections (per atom) for heavy water. In order to obtain cross sections per molecule, one has to multiply by the number of atoms per molecule (i.e., by 3).

		Mixing Fraction	b Fermi	σ_c Barn	$\sigma_{i\text{-spin}}$ Barn	$\sigma_{i\text{-comp}}$ Barn	σ_i Barn	σ_s Barn
Deuterium	D	2/3	6.671	-----	2.05	-----	-----	-----
Oxygen	O	1/3	5.803	-----	0	-----	-----	-----
Heavy Water	D ₂ O	1	6.382	5.118	1.367	0.0210	1.387	6.505

Note that natural hydrogen contains 99.985 % of the H-1 isotope and 0.015 % of the D (or H-2) isotope.

Two quantities are relevant to SANS measurements: the scattering length density that enters in the contrast factor and the macroscopic incoherent scattering cross section which appears as a constant (Q-independent) background. These two quantities are summarized for H₂O and D₂O.

Table 3: Calculated scattering length densities and macroscopic scattering cross sections (per molecule) for water and heavy water.

		v cm ³	b/v Å ⁻²	Σ_c cm ⁻¹	Σ_i cm ⁻¹	Σ_s cm ⁻¹
Water	H ₂ O	$3 \cdot 10^{-23}$	$-5.583 \cdot 10^{-7}$	0.00392	5.608	5.612
Heavy Water	D ₂ O	$3 \cdot 10^{-23}$	$6.382 \cdot 10^{-6}$	0.512	0.139	0.651

The measured and calculated total cross section ($\Sigma_T = \Sigma_s + \Sigma_a$) for H₂O and D₂O are included in a table for thermal neutrons (wavelength of $\lambda = 1.8$ Å). Note that the absorption cross sections are small. Cross sections were obtained from the Evaluated Nuclear Data File (ENDF) online database. This is the so-called “Barn Book”.

Table 4: Measured and calculated macroscopic cross sections for H₂O and D₂O for thermal neutrons

	Σ_T Measured	Σ_T Calculated
H ₂ O	3.7 cm ⁻¹	5.612 cm ⁻¹
D ₂ O	0.49 cm ⁻¹	0.651 cm ⁻¹

The calculated and measured values are different for a number of reasons including the neglect of inelastic scattering effects.

10. GENERAL CASE

Consider the general case of a molecule A_{n_A}B_{n_B}C_{n_C}... containing n_A atoms of element A, etc. The total number of atoms per molecule is $n = n_A + n_B + n_C \dots$ and the number fractions are $f_A = n_A/n$, etc.

The scattering length density is given by:

$$\left(\frac{b}{v}\right) = \frac{n_A b_A + n_B b_B + n_C b_C \dots}{v} \quad (25)$$

Here v is the molecular volume and $b_A, b_B, b_C \dots$ are the tabulated scattering lengths.

The macroscopic scattering cross section is given by:

$$\Sigma_i = \left(\frac{N}{V} \right) ([\sigma_i]_{\text{spin}} + [\sigma_i]_{\text{comp}}) \quad (26)$$

N is the number of molecules in the sample of volume V. The spin incoherence and composition incoherence microscopic cross sections per molecule are given by:

$$[\sigma_i]_{\text{spin}} = n[f_A \sigma_i(A) + f_B \sigma_i(B) + f_C \sigma_i(C) \dots] \quad (27)$$

$$[\sigma_i]_{\text{comp}} = n[\{b^2\} - \{b\}^2] \quad (28)$$

$$[\sigma_i]_{\text{comp}} = n[f_A b_A^2 + f_B b_B^2 + f_C b_C^2 \dots - (f_A b_A + f_B b_B + f_C b_C \dots)^2]$$

$$[\sigma_i]_{\text{comp}} = n[f_A f_B (b_A - b_B)^2 + f_A f_C (b_A - b_C)^2 + f_B f_C (b_B - b_C)^2 \dots]$$

The relation $f_A + f_B + f_C \dots = 1$ has been used. For pure substances, the molecules number density is $(N/V) = 1/v$ where v is the molecular volume given by:

$$v = \frac{m}{N_{\text{av}} d} \quad (29)$$

m and d are the molecular mass and mass density and N_{av} is Avogadro's number.

11. TABULATED SCATTERING LENGTHS AND CROSS SECTIONS

The coherent and incoherent thermal neutron scattering lengths and cross sections are tabulated here for a few elements (Koester, 1991; Sears, 1992). That table also contains the absorption cross section σ_a for thermal neutrons (i.e., with a wavelength of $\lambda = 1.8 \text{ \AA}$ or a kinetic energy of 0.025 eV). Neutron absorption is small for most elements except for boron, cadmium and gadolinium (that are used as neutron absorbers). The absorption cross section is related to the imaginary part b_a of the scattering length $b - ib_a$. Only neutron absorbing materials have an imaginary part. The absorption cross section is expressed as

$$\sigma_a = \frac{4\pi\{b_a\}}{k} \quad (30)$$

k is the incident neutrons wavenumber $k = mv/\hbar$ where \hbar is Planck's constant, m is the neutron mass and v is the incident neutron speed. $\{b_a\}$ is the composition averaged absorption length. The absorption cross section varies like $\sim 1/v$ where v is the neutron speed. The macroscopic absorption cross section is given by $\Sigma_a = (N/V)\sigma_a = \sigma_a/V_{\text{sp}}$ where (N/V) is the number density and V_{sp} is the specific volume of the material.

Table 5: Coherent and incoherent thermal neutron scattering lengths (b_c and b_i) and cross sections (σ_c and σ_i) as well as absorption cross section (σ_{abs}) for some nuclei. Note that 1 fermi= 10^{-13} cm and 1 barn= 10^{-24} cm².

Element	b Fermi	σ_c Barn	σ_i Barn	σ_s Barn	σ_a Barn
H	-3.739	1.757	80.30	82.057	0.333
D	6.671	5.592	2.05	7.642	0.000
C	6.646	5.550	0.001	5.551	0.003
N	9.36	11.01	0.50	11.51	1.90
O	5.803	4.232	0.000	4.232	0.000
F	5.654	4.232	0.001	4.233	0.000
Na	3.63	1.66	1.62	3.28	0.530
Si	4.149	2.163	0.004	2.167	0.171
P	5.13	3.307	0.005	3.312	0.172
S	2.847	1.017	0.007	1.024	0.53
Cl	9.577	11.526	5.3	16.826	33.5

The coherent scattering length for a mixture involves the mean and the incoherent scattering length involves the standard deviation. If one considers a fictitious sample comprising a few low-Z elements in equal amounts, then the deviation from the incoherent scattering length would be the deviation from the average of the scattering lengths plotted vs Z.

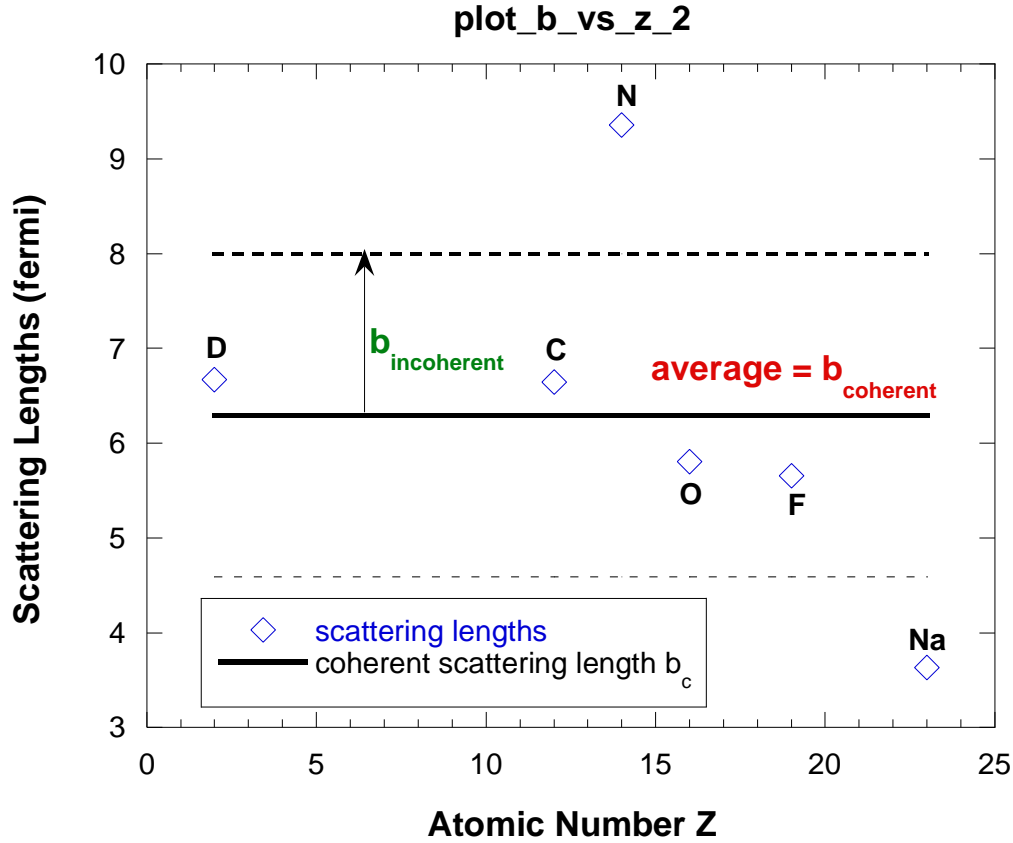


Figure 3: Variation of the scattering length for a few low-Z elements.

12. NEUTRON TRANSMISSION

Neutrons incident on a sample have three choices: they either cross it without interaction, get scattered or get absorbed. Neutron absorption is small for most materials. The neutron transmission of a flat slab sample (appropriate for SANS measurements) of thickness d and total macroscopic cross section:

$$\Sigma_t = \Sigma_s + \Sigma_a = \Sigma_c + \Sigma_i + \Sigma_a \quad (31)$$

is given by:

$$T = \exp(-\Sigma_t d). \quad (32)$$

Here d is the sample thickness. The transmission is measured as the ratio of the direct beam intensity with and without the sample. Transmission gets lower for longer neutron wavelengths.

The total cross section can be estimated in terms of the sample transmission T and sample thickness d as: $\Sigma_t = -\ln(T)/d$. Note that the incoherent component is the dominant form of scattering from samples containing hydrogen in the flat high- Q region.

13. MEASURED MACROSCOPIC CROSS SECTION FOR WATER

Water scatters mostly incoherently and is characterized by a flat (Q -independent) SANS signal. Water is used as a secondary absolute intensity standard since its macroscopic scattering cross section is well known. The SANS measured cross section corresponds to the macroscopic cross section $\Sigma_T/4\pi$. The wavelength-dependent microscopic cross section was obtained from the Evaluated Nuclear Data File (ENDF) online database (the modern version of the so-called Barn Book).

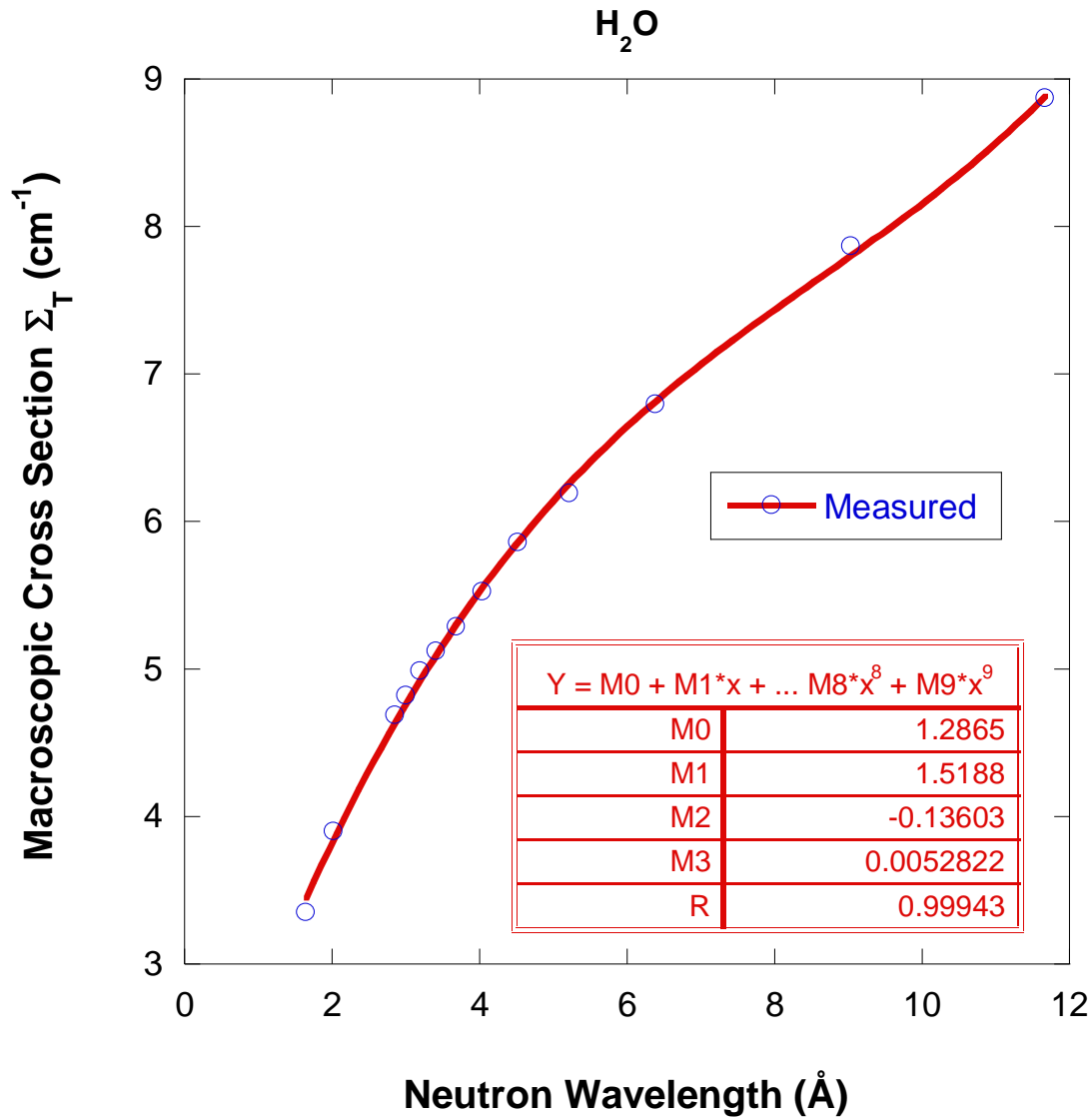


Figure 5: Variation of the **macroscopic cross section Σ_T for H_2O** . Note that the cross section measured by SANS corresponds to $\Sigma_T/4\pi$.

14. CROSS SECTIONS FOR H_2O/D_2O MIXTURES

Often H_2O/D_2O mixtures are used to vary the contrast factor. Ignoring H/D exchange, the variation of the incoherent and coherent microscopic scattering cross sections σ_i and σ_c are summarized. The following scattering lengths and cross sections are used:

$$\begin{aligned} b_H &= 3.739 \text{ fm} \\ b_O &= 5.803 \text{ fm} \\ b_D &= 6.671 \text{ fm} \\ [\sigma_i(H)]_{\text{spin}} &= 80.27 \text{ barn} \\ [\sigma_i(O)]_{\text{spin}} &= 0 \text{ barn} \\ [\sigma_i(D)]_{\text{spin}} &= 2.05 \text{ barn} . \end{aligned} \quad (33)$$

The incoherent cross section is dominated by the spin-incoherent part. Defining the D_2O number fraction (relative number of molecules) as ϕ_{D_2O} in an H_2O/D_2O mixture, the spin-incoherent cross section is given by:

$$\begin{aligned} [\sigma_i(H_2O/D_2O)]_{\text{spin}} &= (1 - \phi_{D_2O})[\sigma_i(H_2O)]_{\text{spin}} + \phi_{D_2O}[\sigma_i(D_2O)]_{\text{spin}} \\ [\sigma_i(H_2O)]_{\text{spin}} &= 160.54 \text{ barn} \\ [\sigma_i(D_2O)]_{\text{spin}} &= 4.10 \text{ barn} \\ [\sigma_i(H_2O/D_2O)]_{\text{spin}} &= 160.54 * (1 - \phi_{D_2O}) + 4.10 * \phi_{D_2O} \text{ barn} . \end{aligned} \quad (34)$$

There are two levels of composition-incoherence; one for disorder within the (H_2O or D_2O) molecules and one for disorder in the H_2O/D_2O mixture. Contribution to the disorder within the molecules is given by:

$$\begin{aligned} [\sigma_i(H_2O)]_{\text{comp}} &= 4\pi \frac{2}{3} (b_H - b_O)^2 = 7.63 \text{ barn} \\ [\sigma_i(D_2O)]_{\text{comp}} &= 4\pi \frac{2}{3} (b_D - b_O)^2 = 0.063 \text{ barn} . \end{aligned} \quad (35)$$

This is the cross section “per molecule”. Contribution to the composition incoherence for the H_2O/D_2O mixture is given by:

$$\begin{aligned} [\sigma_i(H_2O/D_2O)]_{\text{comp}} &= 4\pi (1 - \phi_{D_2O})\phi_{D_2O} [b_{D_2O} - b_{H_2O}]^2 + \\ &\quad \phi_{D_2O} [\sigma_i(D_2O)]_{\text{comp}} + (1 - \phi_{D_2O}) [\sigma_i(H_2O)]_{\text{comp}} \end{aligned} \quad (36)$$

$$[b_{D_2O} - b_{H_2O}]^2 = 4[b_H - b_D]^2 = 4.33 \text{ barn} .$$

Gathering the terms, one obtains:

$$[\sigma_i(H_2O/D_2O)]_{\text{comp}} = (1 - \phi_{D_2O})\phi_{D_2O} 54.47 + \phi_{D_2O} 0.063 + (1 - \phi_{D_2O}) 7.63 \text{ barn} \quad (37)$$

The total incoherent cross section is the sum of the two (spin- and composition-incoherent) contributions. It is equal to:

$$[\sigma_i(H_2O/D_2O)] = (1 - \phi_{D_2O})\phi_{D_2O} 54.47 + \phi_{D_2O} 4.16 + (1 - \phi_{D_2O}) 168.17 \text{ barn} .$$

The coherent scattering cross section for the mixture is given by:

$$\begin{aligned} \sigma_c &= 4\pi * 3 \left[(1 - \phi_{D_2O})b_{H_2O} + \phi_{D_2O}b_{D_2O} \right]^2 \\ \sigma_c &= 0.117 (1 - \phi_{D_2O}) + 15.35 \phi_{D_2O} + 1.342 \phi_{D_2O} (1 - \phi_{D_2O}) \text{ barn} . \end{aligned} \quad (38)$$

The scattering length density for the H₂O/D₂O mixture is given by:

$$\begin{aligned} \rho &= (1 - \phi_{D_2O})\rho_{H_2O} + \phi_{D_2O}\rho_{D_2O} \\ \rho_{H_2O} &= -5.6 * 10^{-7} \text{ \AA}^{-2} \\ \rho_{D_2O} &= 6.4 * 10^{-6} \text{ \AA}^{-2} . \end{aligned} \quad (39)$$

The incoherent and coherent cross sections and the scattering length density are plotted using different scales.

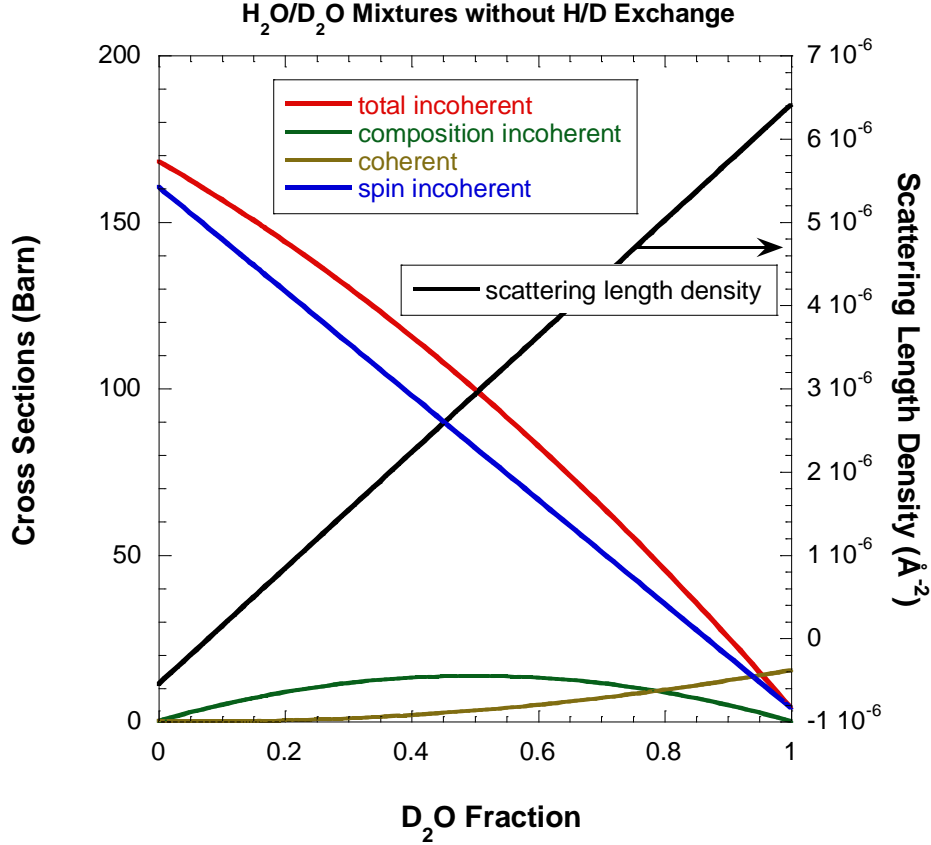


Figure 6: Incoherent and coherent microscopic scattering cross sections for H₂O/D₂O mixtures without D/H exchange.

Now assume that there is full H/D exchange to the point that the H₂O/D₂O/HDO mixture is randomized. The relative fraction of D₂O molecules in the mixture is $\phi_{D_2O}^2$. This is the probability of picking out a pair of D atoms from the randomized H/D mixture. The relative fraction of H₂O molecules is $(1-\phi_{D_2O})^2$ and the relative fraction of HOD and DOH molecules is $2\phi_{D_2O}(1-\phi_{D_2O})$.

With full H/D exchange, the spin-incoherent cross section is the same before and after exchange.

$$\begin{aligned}
 [\sigma_i]_{\text{spin}} &= \phi_{D_2O} [\sigma_i(D_2O)]_{\text{spin}} + (1-\phi_{D_2O}) [\sigma_i(H_2O)]_{\text{spin}} \\
 [\sigma_i]_{\text{spin}} &= \phi_{D_2O}^2 [\sigma_i(D_2O)]_{\text{spin}} + (1-\phi_{D_2O})^2 [\sigma_i(H_2O)]_{\text{spin}} + 2\phi_{D_2O}(1-\phi_{D_2O}) [\sigma_i(DOH)]_{\text{spin}}
 \end{aligned}
 \tag{40}$$

$$[\sigma_i(DOH)]_{\text{spin}} = 82.32 \text{ barn}$$

$$[\sigma_i]_{\text{spin}} = 4.10 * \phi_{D_2O}^2 + 160.54 * (1-\phi_{D_2O})^2 + 164.64 \phi_{D_2O} (1-\phi_{D_2O}) \text{ barn} .$$

Here also, there are two levels of disorder; one within the molecules and one for the molecular mixture. The composition-incoherent cross section becomes:

$$\begin{aligned} [\sigma_i(\text{H}_2\text{O}/\text{D}_2\text{O})]_{\text{comp}} = & 4\pi \left\{ \phi_{\text{D}_2\text{O}}^2 (1 - \phi_{\text{D}_2\text{O}})^2 [\text{b}_{\text{D}_2\text{O}} - \text{b}_{\text{H}_2\text{O}}]^2 + \right. \\ & \phi_{\text{D}_2\text{O}}^2 2\phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) [\text{b}_{\text{D}_2\text{O}} - \text{b}_{\text{HOD}}]^2 + \\ & (1 - \phi_{\text{D}_2\text{O}})^2 2\phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) [\text{b}_{\text{H}_2\text{O}} - \text{b}_{\text{HOD}}]^2 + \\ & \left. \phi_{\text{D}_2\text{O}}^2 [\sigma_i(\text{D}_2\text{O})]_{\text{comp}} + (1 - \phi_{\text{D}_2\text{O}})^2 [\sigma_i(\text{H}_2\text{O})]_{\text{comp}} + 2\phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) [\sigma_i(\text{HOD})]_{\text{comp}} \right\} \end{aligned} \quad (41)$$

Note that:

$$\begin{aligned} [\text{b}_{\text{D}_2\text{O}} - \text{b}_{\text{H}_2\text{O}}]^2 &= 4[\text{b}_{\text{D}} - \text{b}_{\text{H}}]^2 \\ [\text{b}_{\text{D}_2\text{O}} - \text{b}_{\text{HOD}}]^2 &= [\text{b}_{\text{D}} - \text{b}_{\text{H}}]^2 \\ [\text{b}_{\text{H}_2\text{O}} - \text{b}_{\text{HOD}}]^2 &= [\text{b}_{\text{D}} - \text{b}_{\text{H}}]^2 \\ [\sigma_i(\text{DOH})]_{\text{comp}} &= 4\pi \frac{1}{3} [(\text{b}_{\text{D}} - \text{b}_{\text{O}})^2 + (\text{b}_{\text{H}} - \text{b}_{\text{O}})^2 + (\text{b}_{\text{D}} - \text{b}_{\text{H}})^2] = 8.38 \text{ barn} . \end{aligned} \quad (42)$$

After manipulations,

$$\begin{aligned} [\sigma_i(\text{H}_2\text{O}/\text{D}_2\text{O})]_{\text{comp}} = & 4\pi \left\{ (1 - \phi_{\text{D}_2\text{O}}) \phi_{\text{D}_2\text{O}} 2[\text{b}_{\text{D}} - \text{b}_{\text{H}}]^2 + \right. \\ & \phi_{\text{D}_2\text{O}}^2 \frac{2}{3} [\text{b}_{\text{D}} - \text{b}_{\text{O}}]^2 + (1 - \phi_{\text{D}_2\text{O}})^2 \frac{2}{3} [\text{b}_{\text{H}} - \text{b}_{\text{O}}]^2 + \\ & \left. 2\phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) \left(\frac{1}{3} [\text{b}_{\text{D}} - \text{b}_{\text{O}}]^2 + \frac{1}{3} [\text{b}_{\text{H}} - \text{b}_{\text{O}}]^2 + \frac{1}{3} [\text{b}_{\text{H}} - \text{b}_{\text{O}}]^2 \right) \right\} \end{aligned} \quad (43)$$

$$\begin{aligned} [\sigma_i(\text{H}_2\text{O}/\text{D}_2\text{O})]_{\text{comp}} = & 27.23 (1 - \phi_{\text{D}_2\text{O}}) \phi_{\text{D}_2\text{O}} + 0.063 \phi_{\text{D}_2\text{O}}^2 + \\ & 7.63 (1 - \phi_{\text{D}_2\text{O}})^2 + 16.77 \phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) \text{ barn} . \end{aligned}$$

The total incoherent cross section is the sum of the two (spin- and composition-incoherent) contributions. It is equal to:

$$[\sigma_i(\text{H}_2\text{O}/\text{D}_2\text{O})] = 4.16 * \phi_{\text{D}_2\text{O}}^2 + 168.17 * (1 - \phi_{\text{D}_2\text{O}})^2 + 181.41 \phi_{\text{D}_2\text{O}} (1 - \phi_{\text{D}_2\text{O}}) \text{ barn} \quad (44)$$

Including full H/D exchange, the coherent scattering cross section becomes:

$$\sigma_c = 4\pi * 3 \left[(1 - \phi_{\text{D}_2\text{O}})^2 \text{b}_{\text{H}_2\text{O}} + \phi_{\text{D}_2\text{O}}^2 \text{b}_{\text{H}_2\text{O}} + 2(1 - \phi_{\text{D}_2\text{O}}) \phi_{\text{D}_2\text{O}} \text{b}_{\text{HOD}} \right]^2 . \quad (45)$$

This expression can be shown to reduce to the one obtained without D/H exchange:

$$\sigma_c = 4\pi * 3 \left[(1 - \phi_{D_2O}) b_{H_2O} + \phi_{D_2O} b_{H_2O} \right]^2 \quad (46)$$

$$\sigma_c = 0.117 (1 - \phi_{D_2O}) + 15.35 \phi_{D_2O} + 1.342 \phi_{D_2O} (1 - \phi_{D_2O}) \text{ barn} .$$

The scattering length density for the H₂O/D₂O mixture becomes:

$$\rho = (1 - \phi_{D_2O})^2 \rho_{H_2O} + \phi_{D_2O}^2 \rho_{H_2O} + 2\phi_{D_2O} (1 - \phi_{D_2O}) \rho_{HDO} \quad (47)$$

$$\rho_{HDO} = 2.92 * 10^{-6} \text{ \AA}^{-2} .$$

Here also, the incoherent and coherent cross sections and the scattering length density are plotted for the case of full H/D exchange.

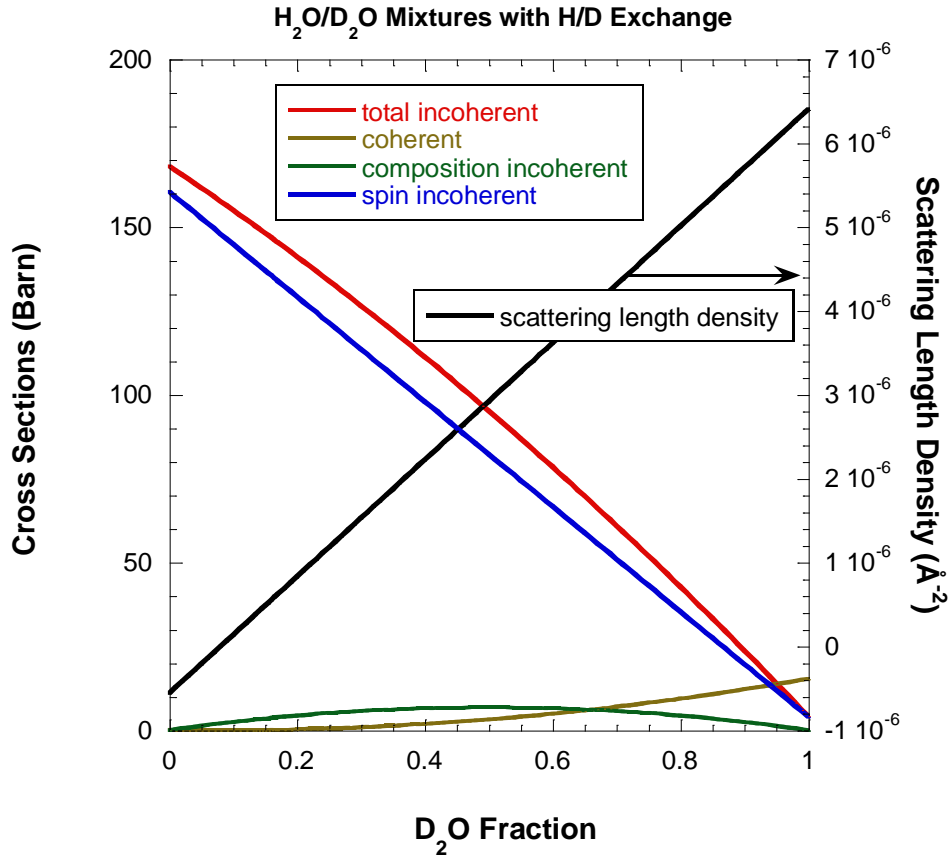


Figure 7: Incoherent and coherent microscopic scattering cross sections for H₂O/D₂O mixtures with full D/H exchange.

Note that just like the incoherent scattering cross section, the isothermal compressibility contribution is also Q-independent but is small.

REFERENCES

L. Koester, H. Rauch, and E. Seymann, "Neutron Scattering Lengths: a Survey of Experimental Data and Methods", Atomic Data and Nuclear Data Tables 49, 65 (1991)

V.F. **Sears**, "Neutron Scattering Lengths and Cross Sections", Neutron News 3, 26-37 (1992).

The Barn Book, Evaluated Nuclear Data File online database is found at the following web address <http://www.nndc.bnl.gov/exfor7/endl00.htm>.

A scattering length density calculator can be found online at:
<http://www.ncnr.nist.gov/resources/sldcalc.html>

QUESTIONS

1. **Neutrons are scattered by what part of the atom?**
2. Are higher fluxes achieved in research reactors (neutron sources) or in synchrotron x-ray sources?
3. **Is deuteration always needed for neutron scattering?**
4. What is the origin of the name for neutron cross sections (barn)?
5. Work out the relative composition of an H₂O/D₂O mixture that would have zero average coherent cross section (so called semi-transparent mixture).
6. **Comparing the coherent scattering cross sections for a deuterated polymer in hydrogenated solvent and a hydrogenated polymer in deuterated solvent, which one has the highest signal-to-noise ratio for dilute solutions?**
7. **Why does carbon have a negligible incoherent scattering cross section?**
8. **What is the meaning of a negative scattering length?**
9. Work out the scattering contrast for a mixture of your choice (or of your own research interest).
10. Calculate the incoherent microscopic scattering cross section per molecule for H₂O.
11. **Define the neutron transmission for a SANS sample. Does it depend on neutron wavelength?**

ANSWERS

1. **Neutrons are scattered by the nuclei.**
2. Synchrotron x-ray sources have much higher fluxes than neutron sources.
3. **Deuteration is not always needed for neutron scattering.** Many systems are characterized by "natural contrasts". Deuteration is however necessary to enhance the contrast of specific structures.
4. The word barn was first used by Fermi in 1942 when initial measurements came up with estimates for the size of neutron-nuclear cross sections. These estimates were larger than expected (as large as a barn!). $1 \text{ barn} = 10^{-24} \text{ cm}^2$. $1 \text{ fm}^2 = 10^{-26} \text{ cm}^2$ was expected.

5. The scattering length density for H₂O (density = 1 g/cm³) is $-5.6 \times 10^{-7} \text{ \AA}^{-2}$. The scattering length density for D₂O (density = 1.11 g/cm³) is $6.38 \times 10^{-6} \text{ \AA}^{-2}$. The H₂O/D₂O mixture that would give zero scattering length density corresponds to 92 % H₂O and 8 % D₂O.
6. The contrast factor is the same for the two systems: deuterated polymer in hydrogenated solvent and hydrogenated polymer in a deuterated solvent (this is the so-called Babinet principle). However, for dilute polymer solutions the level of incoherent scattering background is lower when the solvent is deuterated. The signal to noise (contrast factor/incoherent background level) is higher when deuterated solvent and hydrogenated polymer is used.
7. Carbon has a negligible incoherent scattering cross section because it has zero spin and therefore no spin-incoherence.
8. A negative scattering length (such as in the case of H) means that the phase of the eigenfunction (solution of the Schrodinger equation) is shifted by 180 ° during the scattering process.
9. Consider the polymer solution comprising poly(ethylene oxide) or hPEO in d-water or D₂O. The following calculates the scattering lengths b, scattering length densities b/v and then the contrast factor. The specific volume v is needed in each case.
- hPEO: C₂H₄O, $b_{\text{hPEO}} = 4.139 \times 10^{-13} \text{ cm}$, $v_{\text{hPEO}} = 38.94 \text{ cm}^3/\text{mol}$
d-water: D₂O, $b_{\text{D}_2\text{O}} = 19.14 \times 10^{-13} \text{ cm}$, $v_{\text{D}_2\text{O}} = 18 \text{ cm}^3/\text{mol}$
Contrast Factor: $(b_{\text{hPEO}}/V_{\text{hPEO}} - b_{\text{D}_2\text{O}}/v_{\text{D}_2\text{O}})^2 N_{\text{av}} = 5.498 \times 10^{-3} \text{ mol/cm}^4$, N_{av} is Avogadro's number.
10. Use the standard expression for the cross section per atom $\sigma_{\text{incoh}}(\text{H}_2\text{O}) = 4\pi f_{\text{H}} f_{\text{O}} (b_{\text{H}} - b_{\text{O}})^2 + f_{\text{H}} \sigma_{\text{incoh}}(\text{H}) + f_{\text{O}} \sigma_{\text{incoh}}(\text{O})$ where $b_{\text{H}} = -3.739 \text{ fm}$ and $b_{\text{O}} = 5.803 \text{ fm}$ are the coherent scattering lengths for H and O, $\sigma_{\text{incoh}}(\text{H}) = 80.27 \text{ barn}$ and $\sigma_{\text{incoh}}(\text{O}) = 0 \text{ barn}$ are the spin-incoherent scattering cross sections and $f_{\text{H}} = 2/3$ and $f_{\text{O}} = 1/3$ are the relative number fractions. Note that $1 \text{ fm} = 10^{-13} \text{ cm}$ and $1 \text{ barn} = 10^{-24} \text{ cm}^2$. The result for the cross section per atom is $\sigma_{\text{incoh}}(\text{H}_2\text{O}) = 56 \text{ barn}$. The cross section per molecule is $3\sigma_{\text{incoh}}(\text{H}_2\text{O}) = 168 \text{ barn}$.
11. The SANS transmission from a flat sample of thickness d and total macroscopic scattering cross section Σ_t is given by $T = \exp(-\Sigma_t d)$. Transmission decreases with increasing neutron wavelength.